The oxidation of furfural in a jet-stirred reactor: a combined experimental and modeling approach

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The fast pyrolysis of biomass is a trendy topic in recent studies regarding the need for fuels and chemicals from renewable resources. Furfural is identified as one of the major compounds produced during the pyrolysis of biomass. Only one experimental study on furfural oxidation is reported by Thorton et al. in a jet-stirred stirred reactor at temperatures of 1000-1300 K. This dataset is limited to higher temperatures and does not include the initial oxidation products of furfural. For this reason, the oxidation of furfural is studied in a jet-stirred reactor at atmospheric pressure and temperatures of 600-1000 K. Stoichiometric (ϕ=1.0) and fuel-lean (ϕ=0.5) conditions are considered for an average residence time of 2s and a furfural inlet mole fraction of 0.005.

The conversion of furfural starts at 725 K and 675 K for ϕ=1.0 and 0.5 respectively. As expected from the molecular structure of furfural, no low-temperature oxidation is observed. Theoretical calculations have confirmed that, after the addition of molecular oxygen to the furfural radicals, the barrier for isomerization is similar to or higher than the re-dissociation channel. The main intermediate species detected are lactones. The mole fraction profiles of these species as a function of temperature are given in the figure. Automatic kinetic model generation together with theoretical calculations will be used to find the most important pathways for the formation of these intermediates and other final oxidation products.

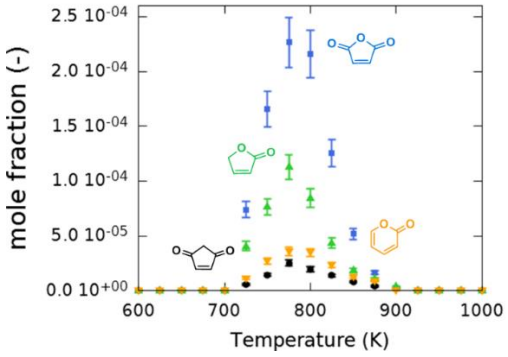

Figure 1. Experimentally measured mole fractions of intermediate species. Experiments are performed in a jet-stirred reactor with $x_{Furfural}$=0.005, ϕ=1.0 and p=1.07 bar.